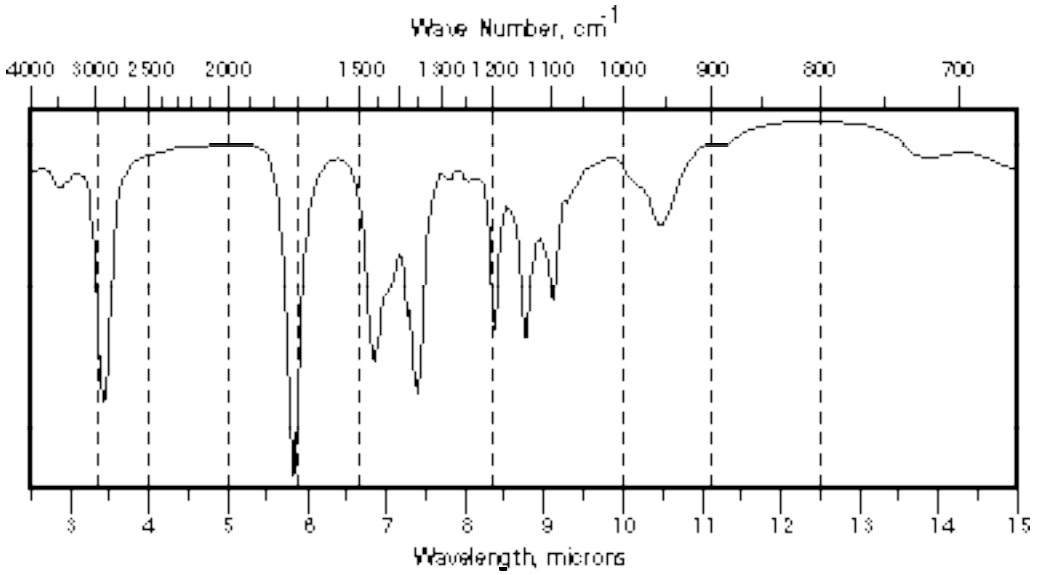
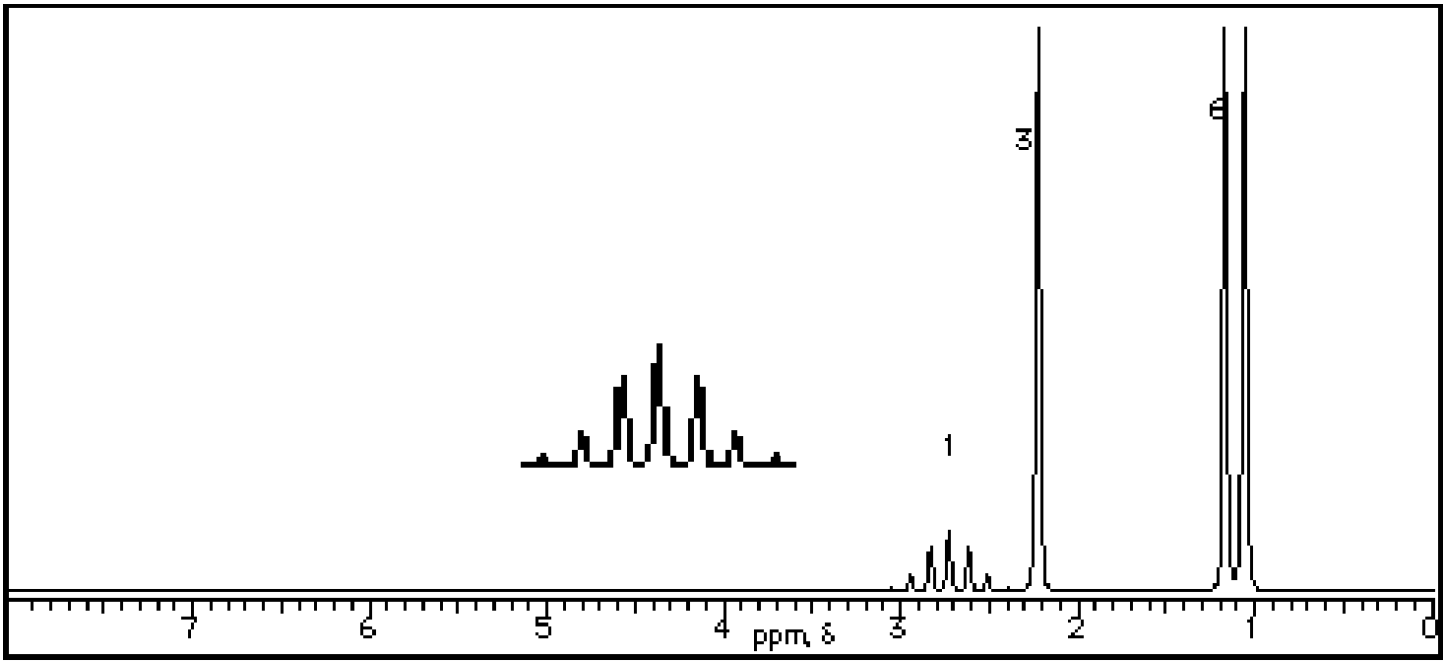
11. Below is the IR and ^{1}H NMR spectra for an unknown compound with a molecular formula $C_5H_{10}O$. In the ^{13}C NMR, four resonances appear at 210, 45, 22, and 16 ppm.

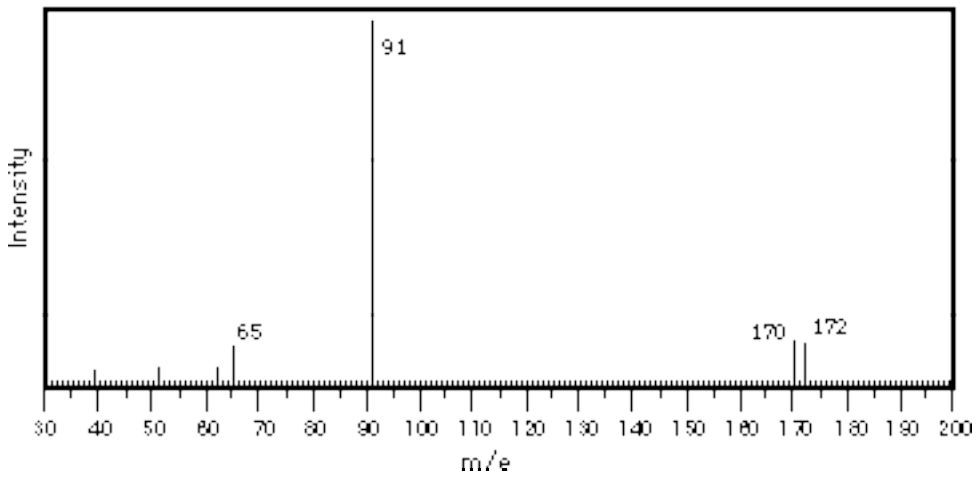




(a) The IR stretching frequency at 1720 cm^{-1} corresponds to what functional group? (4 points)

(b) What is the structure of this molecule? (8 points)

12. A molecule with the molecular formula C_7H_7Br displays the following mass spectrum.



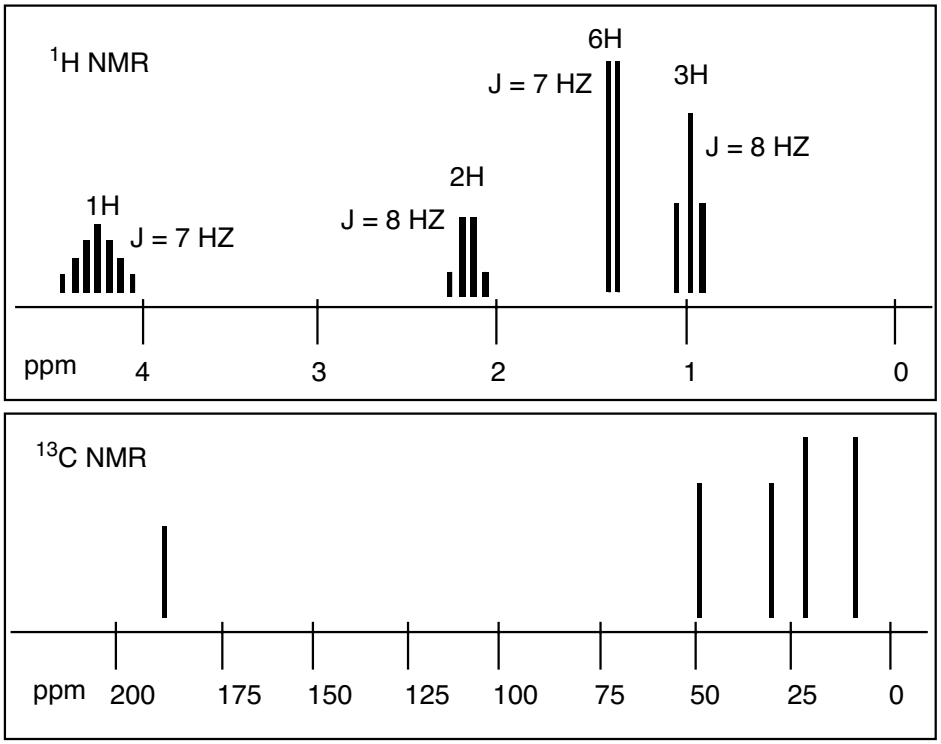
(a) How many units of unsaturation are present? (3 points)

(b) What is the structure of the base peak at m/e 91? (3 points)

(c) What is the structure of the molecule? (3 points)

(d) Briefly explain why there are two peaks at m/e 170 and 172 of nearly equal amounts. (3 pts)

6) A molecule with the formula $C_6H_{12}O_2$ shows a characteristic Infrared absorption at 1735 cm^{-1} and the following NMR spectra. The proton spectra shows the peaks, the number of hydrogens that each resonance integrates for, and the coupling constant (J in Hz). The carbon spectrum shows 5 different carbons.

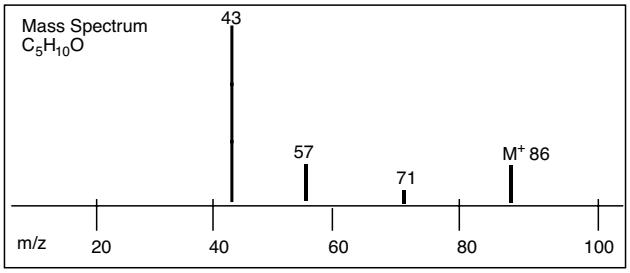


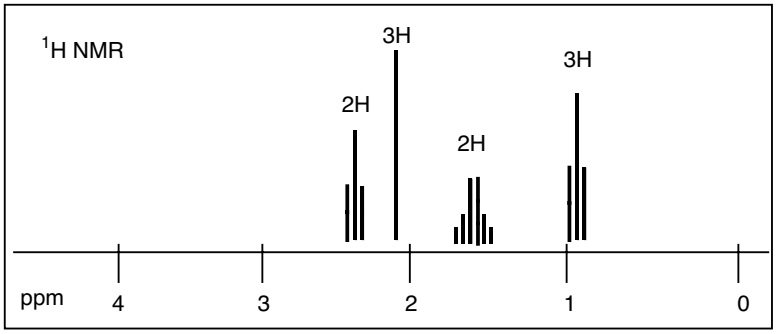
a) Calculate the degrees of unsaturation in this molecule: (5 points)

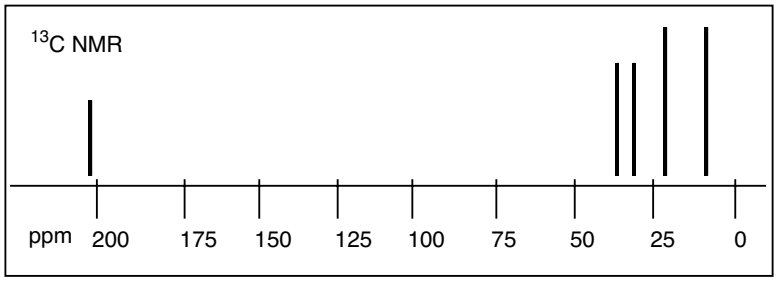
b) What functional group does the IR absorption at 1735 cm^{-1} correspond to? (5 points)

c) Draw the structure of this molecule (partial credit will be given for correct "pieces" of the molecule if they match the NMR data). (15 points)

10) A molecule with the formula $C_5H_{10}O$ shows a characteristic Infrared absorption at 1715 cm^{-1} and the following MS and NMR spectra. The proton spectra shows the peaks and the relative number of hydrogens that each resonance integrates. The carbon spectrum shows 5 different carbons. (33 points)





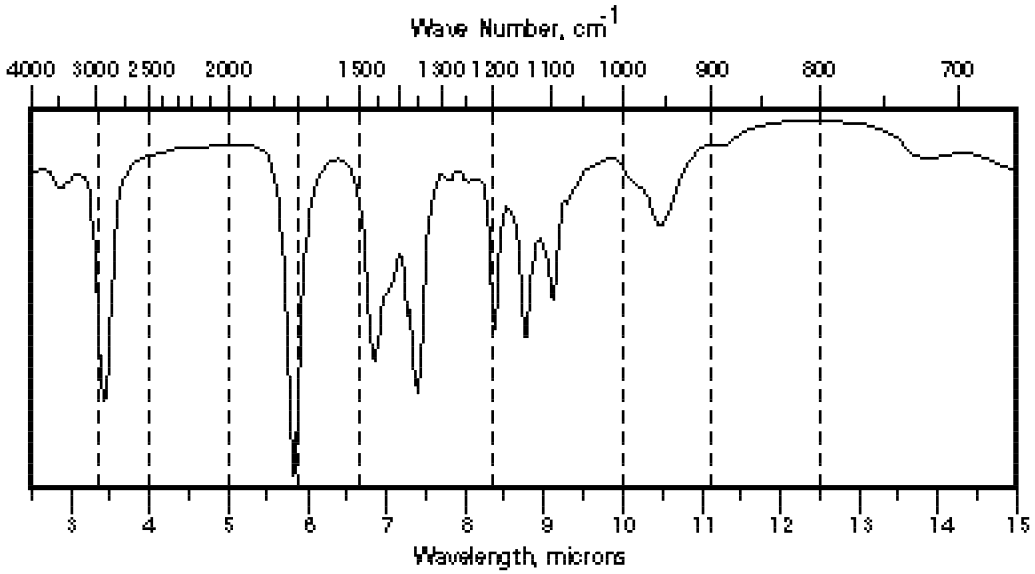


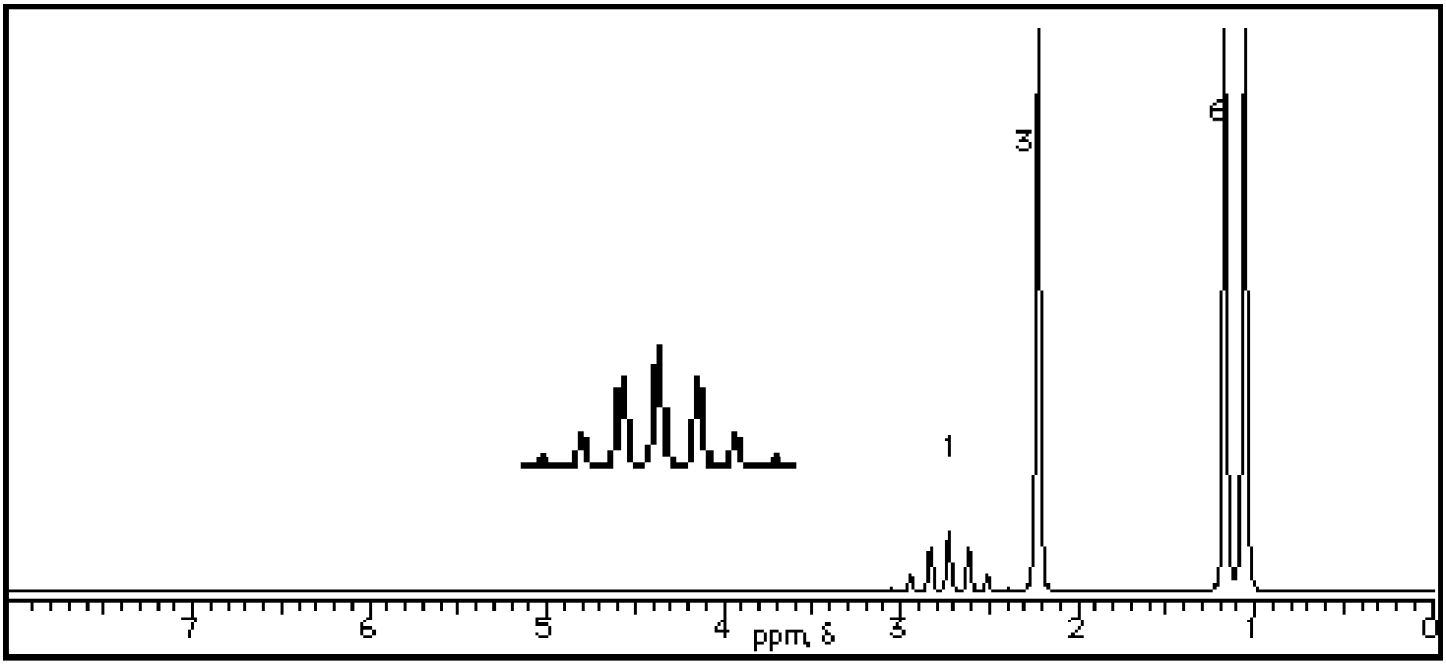
a) What functional group is present in this molecule? (3 points)

b) Draw the structure of this molecule (partial credit will be given for correct "pieces" of the molecule if they match the NMR data). (15 points)

c) What is the structure for the base peak in the Mass Spectrum? Briefly explain why this fragment is particularly stable. (15 points)

11. Below is the IR and ^{1}H NMR spectra for an unknown compound with a molecular formula $C_5H_{10}O$. In the ^{13}C NMR, four resonances appear at 210, 45, 22, and 16 ppm.

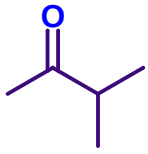




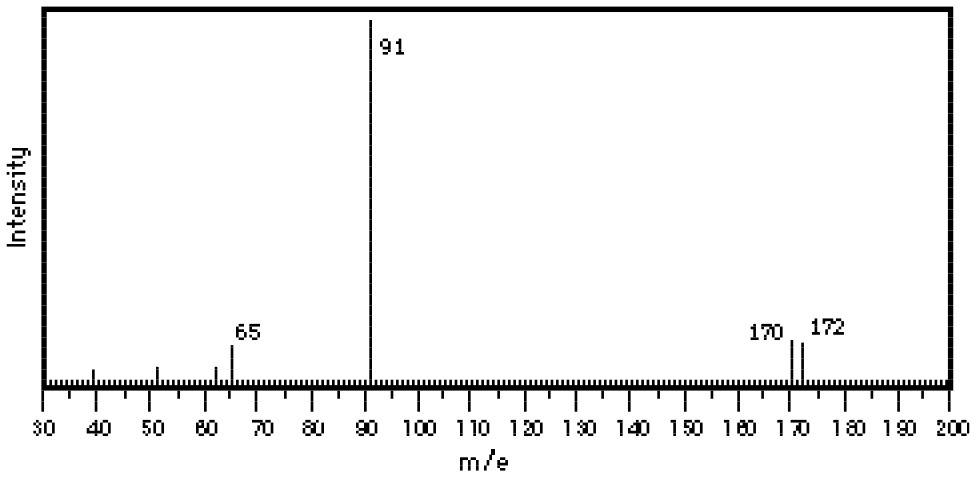
(a) The IR stretching frequency at 1720 cm^{-1} corresponds to what functional group? (4 points)

Carbonyl (Ketone)

(b) What is the structure of this molecule? (8 points)

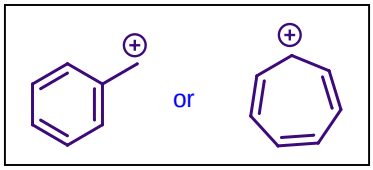


12. A molecule with the molecular formula C_7H_7Br displays the following mass spectrum.

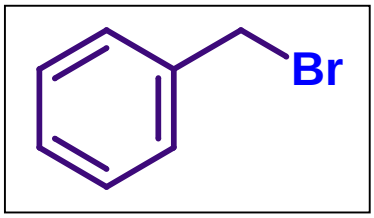


(a) How many units of unsaturation are present? (3 points) **4**

(b) What is the structure of the base peak at m/e 91? (3 points)



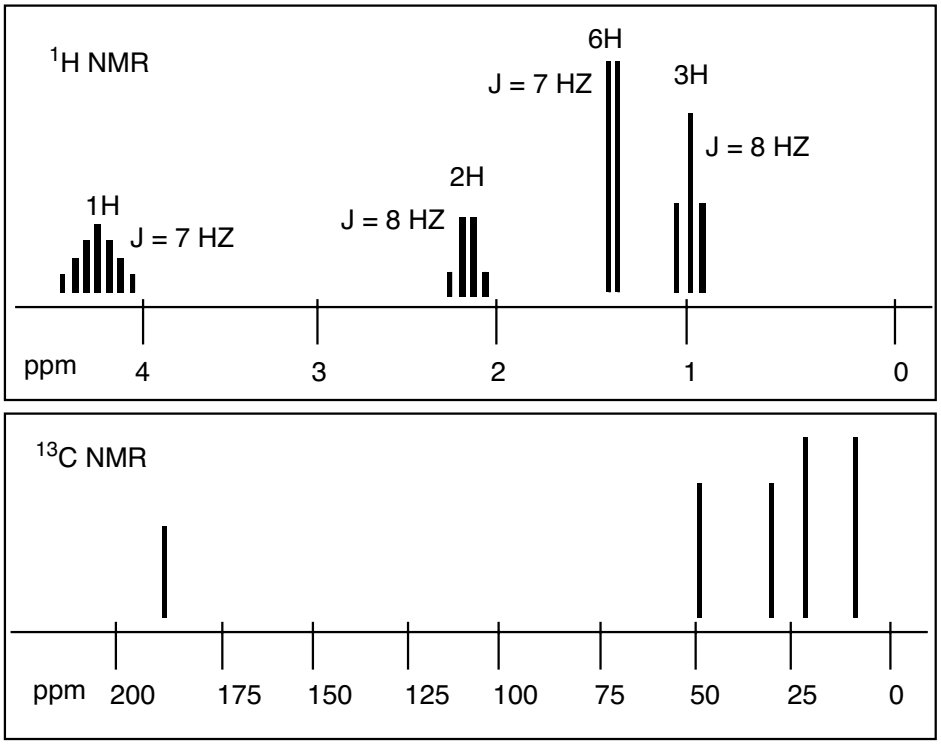
(c) What is the structure of the molecule? (3 points)



(d) Briefly explain why there are two peaks at m/e 170 and 172 of nearly equal amounts. (3 pts)

Bromine exists in nature as roughly a 50:50 mixture of two isotopes which are 2 mass units different.
^{79}Br and ^{81}Br

6) A molecule with the formula $C_6H_{12}O_2$ shows a characteristic Infrared absorption at 1735 cm^{-1} and the following NMR spectra. The proton spectra shows the peaks, the number of hydrogens that each resonance integrates for, and the coupling constant (J in Hz). The carbon spectrum shows 5 different carbons.

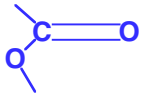


a) Calculate the degrees of unsaturation in this molecule: (5 points)

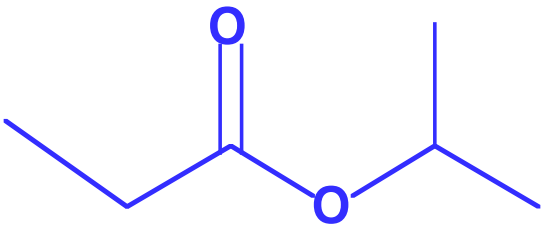
1

b) What functional group does the IR absorption at 1735 cm^{-1} correspond to? (5 points)

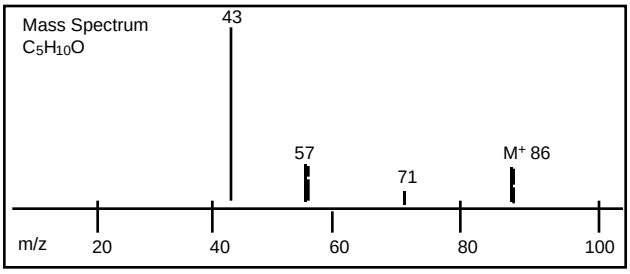
Carbonyl (ester)

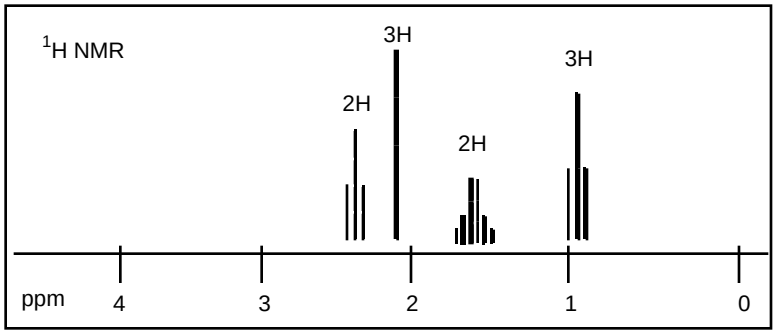


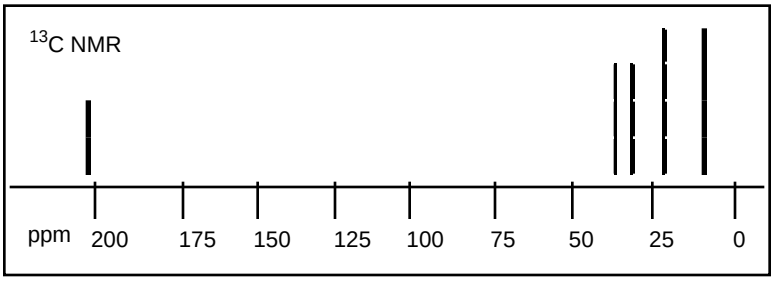
c) Draw the structure of this molecule (partial credit will be given for correct "pieces" of the molecule if they match the NMR data). (15 points)



10) A molecule with the formula $C_5H_{10}O$ shows a characteristic Infrared absorption at 1715 cm^{-1} and the following MS and NMR spectra. The proton spectra shows the peaks and the relative number of hydrogens that each resonance integrates. The carbon spectrum shows 5 different carbons. (33 points)

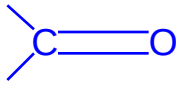




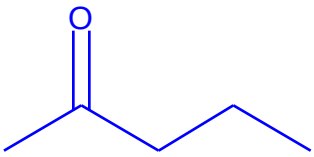


a) What functional group is present in this molecule? (3 points)

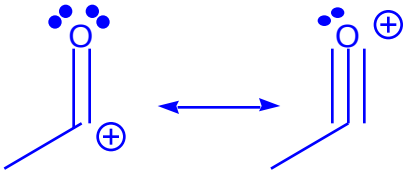
Carbonyl (ketone)



b) Draw the structure of this molecule (partial credit will be given for correct "pieces" of the molecule if they match the NMR data). (15 points)



c) What is the structure for the base peak in the Mass Spectrum? Briefly explain why this fragment is particularly stable. (15 points)



In carbonyl compounds, cleavage to form a cation on the carbonyl carbon is favored because it can be stabilized by resonance with a lone pair on the oxygen.